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Computer modeling is a key tool in understanding wave phenomena in nature. It is used for instance in seismology for exploring the consequences of the Earth's fine structure and in electromagnetism for modeling of radar and microwave signals. Iterative, model driven estimation of material structure and constitutive parameters in an oft-proposed application of computer modeling, but requires very fast simulations to achieve its potential. These simulations are computationally challenging especially in three dimensions.

This project studied a variety of approaches to improving the efficiency and fidelity of wave simulations. It also developed a basic software approach to material parameter estimation. This software is designed, for example, to assis in the interpretation of Ground Penetrating Radar data for civil and environmental engineering applications.

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"Wavelet based projection methods for numerical wave propagation"

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April 20, 2000

Abstract

Computer modeling is a key tool in understanding wave phenomena in nature. It is used for instance in seismology for exploring the consequences of the Earth's fine structure and in electromagnetism for modeling of radar and microwave signals. Iterative, model driven estimation of material structure and constitutive parameters is an oft-proposed application of computer modeling, but requires very fast simulations to achieve its potential. These simulations are computationally challenging especially in three dimensions.

This project studied a variety of approaches to improving the efficiency and fidelity of wave simulations. It also developed a basic software approach to material parameter estimation. This software is designed, for example, to assist in the interpretation of Ground Penetrating Radar data for civil and environmental engineering applications.

Research Topics

Computer modeling is a key tool in understanding wave phenomena in nature. It is used for instance in seismology for exploring the consequences of the Earth's fine structure and in electromagnetism for modeling of radar and microwave signals. Iterative, model driven estimation of material structure and constitutive parameters is an oft-proposed application of computer modeling, but requires very fast simulations to achieve its potential. These simulations are computationally challenging especially in three dimensions.

This project began with the study of a particular simulation approach, which we called the Wavelet/Galerkin method. The use of wavelets as basis function in a Galerkin method leads to explicit time stepping schemes, combining the computational efficency of finite difference methods with the analytical simplicity of finite element methods. We aimed to gain insight into the behaviour of these methods, especially in comparison with standard finite element and finite difference methods for the same problems.

The application of wave modeling to material property estimation formed the other focus of this project, especially the estimation of electromagnetic properties of soil and rock for civil and environmental engineering projects, using Ground Penetrating Radar (GPR). The proposed approach differed from other reported efforts in this topic in the use of a full-blown numerical simulator for radar waves, driving optimization software for data fitting.

Progress in Numerical Wave Simulation

Work complete before the beginning of the project determined that at least a considerable subset of wavelet-Galerkin methods are actually equivalent to explicit finite difference methods, though in some cases with novel choices of stencils, especially for order higher than four. For the application to GPR, we confined our attention for the duration of this project to schemes of order four, hence to standard finite difference methods. Several interesting questions about wavelet-Galerkin methods remain open, and were not addressed in our work, notably whether these methods result in a superior treatment of boundary conditions for systems, such as free surfaces in elastodynamics.

Computation of wave phase without other details of wave motion is possible through solution of the eikonal equation from geometric optics. Finite difference methods developed in the PI's group and elsewhere perform these

calculations with unprecedented efficiency. S. Kim enhanced this efficiency considerably by observing a superconvergence property. Some approaches to material property estimation requires the simulation of the perturbational eikonal equation and its adjoint problem. In carrying out these perturbational and adjoint calculations, A. Sei discovered a disparity between numerical accuracy of the perturbational simulator and the adjoint perturbational simulator, which turns out to be fundamental and unavoidable.

While this project emphasizes broadband GPR, frequency domain simulation and analysis remain relevant for various reasons. S. Kim developed further work begun in his thesis (under Prof. Jim Douglas at Purdue) on domain decomposition for the Helmholtz equation. Finite element and finite difference discretizations of this equation, a prototype for frequency-domain Maxwell, yield very large nonsymmetric illconditioned linear systems, for which standard iterative methods converge slowly or fail to converge altogether. B. Despres pioneered the mathematics of domain decomposition to produce preconditioners for these systems. Kim has answered many questions about the discrete aspects of domain decomposition left open by Despres. He has produced a class of methods with optimal convergence properties, i.e. depending weakly or not at all on discretization, by combining domain decomposition, multigrid, and various Krylov iterations.

Interfaces in Earth materials exist, across which material parameters take large jumps. An example is the water table, at which the speed of compressional seismic waves increases by a factor of up to five, and the electrical conductivity jumps by orders of magnitude in some cases. Finite difference methods are generally subject to degradation of accuracy in the presence of parameter discontinuities such as these. C. Zhang, continuing his thesis work, devised several increasingly sophisticated variants of the *immersed interface method*, which maintains the accuracy of finite difference methods even in the presence of jump discontinuities in parameters. This approach is being further developed by others, and will be very important in realistic modeling of Earth response and estimation of parameters from field measurements.

To initialize the work on GPR imaging, Zhang also produced an overview report summarizing the state of the art in GPR simulation.

The work overviewed in this section is reported in [13, 15, 14, 3, 8, 6, 7, 9, 20, 18, 17, 16, 21, 19]

Progress in Earth parameter estimation

Perturbational and adjoint perturbational computations for wave equations are the drivers of model-based parameter estimation, as envisioned for GPR in the second goal of this project. The construction of these simulators is complicated: several related code modules must function in consort. Especially production of the adjoint code is tedious and error prone. A number of researchers in various areas (for example oceanography and meteorology, where many such simulator-driven parameter estimation problems arise) have developed so called Automatic Differentiation ("AD") software, which automates the production of perturbational and adjoint perturbational code from basic simulator code. Certain technical problems render this automation exceedingly difficult for whole simulators, whereas most of the packages can handle the submodules which implement single steps. This project saw the development of two generations of template code, which fully implements an efficient strategy for perturbational and adjoint code for time stepping methods, except for the single step code, the latter being supplied through use of AD tools. J. Blanch constructed the first, all-Fortran template, and demonstrated its use in the context of viscoacoustic simulation and parameter estimation. C. Zhang and the PI collaborated to develop a second generation object oriented template in C++, which we successfully coupled to Fortran single step code produced by AD tools.

The second generation template actually produces class definitions of operator objects as defined by the Hilbert Class Library ("HCL"), a C++ library for linking complex simulation with optimization code. This library (development of which is supported by continuing grants from NSF and DoE) is designed to overcome a difficulty often faced by scientific programmers, in particular by the investigators in this project. Procedural library code for optimization, linear algebra, etc., however high in quality, is difficult to link to complex simulators, because the latter involve data structures incompatible with the primitive types used by the library code. HCL overcomes these difficulties by separating cleanly the levels of abstraction required by the two types of task (simulation vs. optimization), using object oriented programming techniques.

Zhang completed this construction for TE polarized Maxwell's equations. Unfortunately the project ended before extensive testing of the parameter estimation capabilities of the package could take place. Another very important part of the original agenda which did not receive any useful attention in the

project was antenna modeling. Both of these tasks would need prosecution before any serious evaluation of the proposed approach can be carried out.

The work overviewed in this section is reported in [1, 2, 10, 12, 3, 11, 5, 4]

List of participating scientific personnel

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3. Postdoctoral Associate S. Kim (July 1996 - June 1997; presently Assistant Professor of Mathematics, U. Kentucky, Lexington KY)

4. Postdoctoral Associate C. Zhang (July 1996 - June 1998; presently Western Geophysical, Houston, TX)

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